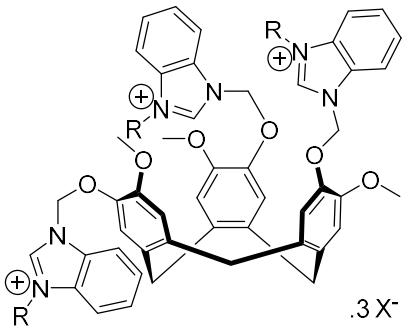
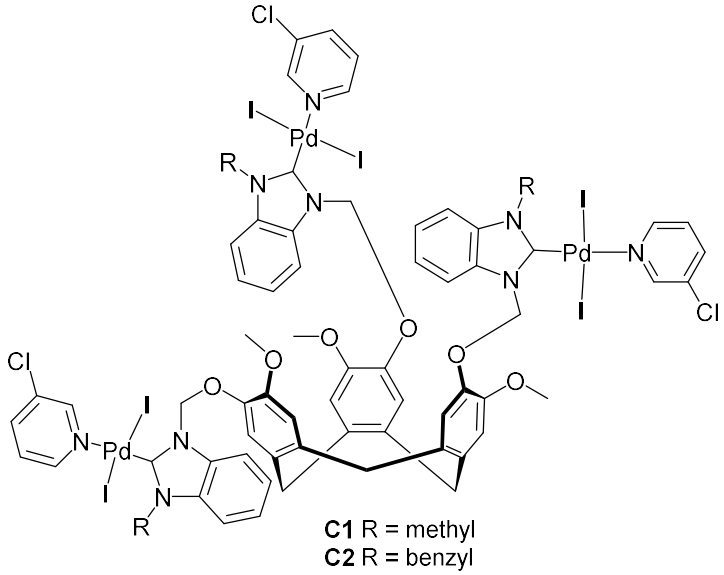
Data refers to the following complexes:

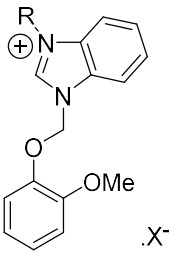


.3 X⁻

R = methyl, $(H_3L1)^{3+}$
R = benzyl, $(H_3L2)^{3+}$

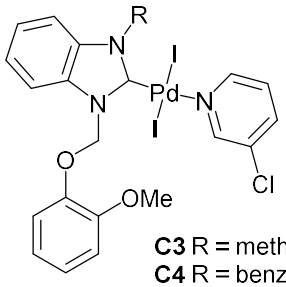


C1 R = methyl
C2 R = benzyl



.X⁻

R = methyl, $(HL3)^{+}$
R = benzyl, $(HL4)^{+}$



C3 R = methyl
C4 R = benzyl

$H_3L1.I_3$ = *tris*-methyl(methylbenzimidazol-1-yl)cyclotriguaiacylenyl iodide,
$H_3L1.(PF_6)_3$ = *tris*-methyl(methylbenzimidazol-1-yl)cyclotriguaiacylenyl hexafluorophosphate,
$H_3L2.I_3$ = tris-benzyl(methylbenzimidazol-1-yl)cyclotriguaiacylenyl iodide
2-(methoxyphenoxymethyl)benzimidazole
HL3.I = 1-(2-methoxyphenyoxy)methyl-3-methylbenzimidazolium iodide
HL4.Br = 1-(2-methoxyphenyoxy)benzyl-3-methylbenzimidazolium bromide
C1 = (±)-tris-(3-chloropyridyl)(methyl(cyclotriguaiacylenyl)methylbenzimidazol-2-ylidene)palladium(II) iodide
C2 = (±)-tris-(3-chloropyridyl)(benzyl(cyclotriguaiacylenyl)methylbenzimidazol-2-ylidene)palladium(II) iodide
C3 = trans-(3-chloropyridyl)-1-(2-methoxyphenyoxy)methyl-3-methylbenzimidazol-2-ylidene palladium(II) iodide
C4 = trans-(3-chloropyridyl)-1-(2-methoxyphenyoxy)methyl-3-benzyllbenzimidazol-2-ylidene palladium(II) iodide

Folder name	Contents
Crystal Structures	Crystallographic Information Files (.cif) with embedded shelxl refinement instructions and hkl data. Observed and calculated structure factor files (.fcf) ligand1 = **$H_3L1.(PF_6)_3$** ligand3 = **HL3.I** complex C1d = [**C1**]$_2$.$^{11}/_2$($C_4H_8O_2$) complex C1p = [**C1**].2(C_5H_{14}).$^1/_2$(CH_2Cl_2).$^3/_2$(H_2O) complex C3 = **C3**

	complex C4 = **C4**
NMR	Raw data and MestReNova files of nuclear magnetic resonance experiments Includes ^{1}H, $^{13}C\{^{1}H\}$, ^{1}H-^{1}H COSY, ^{1}H-^{13}C HMBC + HSQC, ^{13}C DEPT-135 Characterisation of compounds and catalysis studies monitored by ^{1}H NMR
Mass Spec	Mass spectrometry data in pdf format for all listed compounds
Analysis	Infrared spectroscopy spectra as jpg files CHN.pdf - elemental analysis results